Nonexponential decay via tunneling to a continuum of finite width

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A simple quantum mechanical model consisting of a discrete level resonantly coupled to a continuum of finite width, where the coupling can be varied from perturbative to strong, is considered. The particle is initially localized at the discrete level, and the time dependence of the amplitude to find the particle at the discrete level is calculated without resorting to perturbation theory and using only elementary methods. The deviations from the exponential decay law, predicted by the Fermi's Golden Rule, are discussed.

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The transition of a quantum particle from an initial discrete state of energy ϵ into continuum of final states is considered in any textbook on quantum mechanics. It is well known that perturbation theory approach, when used to solve the problem, leads to Fermi's Golden Rule (FGR), which predicts the exponential decrease of the probability to find the particle in the discrete state. It is also well known that, even for a weak coupling between the discreet state and the continuum, this result (exponential decrease of probability) has a finite range of applicability, and is not valid either for very small or for very large time (see e.g. Cohen-Tannoudji et. al. [1]). This complies with the theorem proved 50 years ago, and stating that for quantum system whose energy is bounded from below, i.e., $(0,\infty)$ the exponential decay law cannot hold in the full time interval [2, 3, 4]. The same statement remains valid when the discrete state is coupled to the continuum bounded both from below and above, the model we presently consider. Fortunately, the model is exactly solvable; the solution in the frequency representation obtained within the Green's functions (GF) formalism is presented in [5], where the model is called the Fano-Anderson model). In this paper we solve the problem of tunneling in the framework of Quantum mechanics proper We concentrate on the calculation of the time dependent non-decay amplitude, the stage which is typically not given proper attention to within the GF formalism [5]. We analyze the relation between the exact results and those given by the FGR.

The system consists of the continuum band, the states bearing index k, and the discrete state d. The Hamiltonian of the problem is

$$H=\sum_k \omega_k \left|k\right\rangle\left\langle k\right| + \epsilon\left|d\right\rangle\left\langle d\right| + \sum_k \big(V_k\left|k\right\rangle\left\langle d\right| + h.c.\big), \quad (1)$$

where $|k\rangle$ is the band state and $|d\rangle$ is the state localized at site d; h.c. stands for Hermitian conjugate. The wavefunction can be presented as

$$\psi(t)=g(t)\left|d\right\rangle + \sum_k b(k,t)\left|k\right\rangle, \quad (2)$$

with the initial conditions $a(0)=1$, $b(k,0)=0$. Schroedinger Equation for the model considered takes the form

$$\begin{aligned} i\frac{dg(t)}{dt} &= \epsilon g(t) + \sum_k V_k^* b(k,t) \\ i\frac{db(k,t)}{dt} &= \omega_k b(k,t) + V_k g(t) \end{aligned} \quad (3)$$

Making Fourier transformation (Im $\omega>0$)

$$g(\omega)=\int_0^\infty g(t)e^{i\omega t}dt, \quad (4)$$

we obtain

$$\begin{aligned} -i+\omega g(\omega) &= \epsilon g(\omega) + \sum_k V_k^* b(k,\omega) \\ \omega b(k,\omega) &= \omega_k b(k,\omega) + V_k g(\omega). \end{aligned} \quad (5)$$

For the amplitude to find electron at the discrete level, straightforward algebra gives

$$g(t)=\frac{1}{2\pi i}\int g(\omega)e^{-i\omega t}d\omega, \quad (6)$$

where

$$g(\omega) = \frac{1}{\omega-\epsilon-\Sigma(\omega)} \quad (7)$$

$$\Sigma(\omega) = \sum_k \frac{|V_k|^2}{\omega-\omega_k}, \quad (8)$$

and integration in Eq. (6) is along any infinite straight line parallel to real axis in the upper half plane of the complex ω plane. Notice that if, in addition, we define $g(t)=0$ for $t<0$, then $g(t)$ is just the (single particle in an empty band) GF in time representation, and $g(\omega)$ is the same GF in frequency representation. The quantity $\Sigma(\omega)$ in the GF formalism is called self-energy (or mass operator).

For tunneling into continuum, the sum in Eq. (8) should be considered as an integral, and Eq. (8) takes the form

$$\Sigma(\omega)=\int_{E_b}^{E_t}\frac{\Delta(E)}{\omega-E}dE, \quad (9)$$

where

$$\Delta(E) = \sum_k |V_k|^2 \delta(E - \omega_k), \tag{10}$$

where and the limit of integration are the band bottom E_b and the top of the band E_t. We would like to calculate integral (6) closing the integration contour by a semi-circle of an infinite radius in the lower half-plane. Thus we need to continue analytically the function $g(\omega)$ which was defined initially in the upper half plane (excluding real axis) to the whole complex plane. We can do it quit simply, by considering Eqs. (7) and (9) as defining propagator in the whole complex plane, save an interval of real axis between the points E_b and E_t, where Eq. (9) is undetermined. (Propagator analytically continued in such a way we'll call the standard propagator.) Thus the integral is determined by the integral of the sides of the branch cut between the points E_b and E_t. The real part

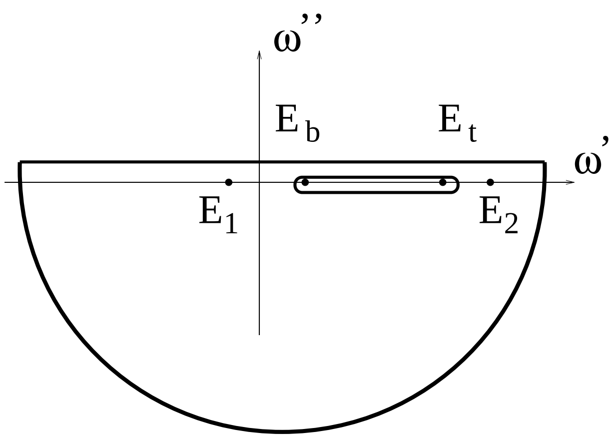


FIG. 1: Contour used to evaluate integral (6). Radius of the arc goes to infinity.

of the self-energy Σ' is continuous across the cut, and the imaginary part Σ'' changes sign

$$-\Sigma''(E + is) = \Sigma''(E - is) = \pi\Delta(E) \quad s \to +0. \tag{11}$$

So the integral along the branch cut is

$$I_{cut} = \int_{E_b}^{E_t} \frac{\Delta(E) e^{-iEt} dE}{[E - \epsilon - \Sigma'(E)]^2 + \pi^2\Delta^2(E)}. \tag{12}$$

Thus we have

$$g(t) = I_{cut}(t), \tag{13}$$

and the survival probability $p(t)$ is

$$p(t) = |g(t)|^2. \tag{14}$$

In the perturbative regime $|\Sigma'(\epsilon)|, |\Sigma''(\epsilon)| \ll \epsilon - E_b, E_t - \epsilon$ the main contribution to the integral (12) comes from the region $E \sim \epsilon$. Hence the integral can be presented as

$$I_{cut} = \int_{-\infty}^{\infty} \frac{\Delta(\epsilon) e^{-iEt} dE}{(E - \epsilon)^2 + \pi^2\Delta^2(\epsilon)} \tag{15}$$

and easily calculated to give the well known Fermi's golden rule (FGR)

$$p(t) = e^{-t/\tau}, \tag{16}$$

where

$$1/\tau = 2\pi\Delta(\epsilon). \tag{17}$$

However, even in perturbative regime, the FGR has a limited time-domain of applicability [1]. For large t the survival probability is determined by the contribution to the integral (12) coming from the end points. This contribution can be evaluated even without assuming that the coupling is perturbative. Let near the band bottom (the contribution from the other end point is similar) $\Delta(E) \sim (E - E_b)^\beta$, where $\beta > 0$. Then for large t

$$I_{cut}^{(b)} \sim t^{-(\beta+1)}. \tag{18}$$

The similar contribution comes from the top of the band.

If there can exist poles of locator (7), we should add to the integral (12) the residues

$$g(t) = I_{cut}(t) + \sum_j R_j, \tag{19}$$

where the index j enumerates all the real poles E_j of the integrand, and

$$R_j = \frac{e^{-iE_j t}}{1 - \frac{d\Sigma'}{dE}\Big|_{E=E_j}}. \tag{20}$$

Notice, that the poles correspond to the energies of bound states which can possibly occur for $E < E_b$ or $E > E_t$, and which are given by the Equation

$$E_j = \epsilon + \sum_k \frac{|V_k|^2}{\omega - \omega_k}. \tag{21}$$

If we take into account that normalized bound states are

$$|E_j\rangle = \frac{|d\rangle + \sum_k \frac{V_k}{E_j - \omega_k} |d\rangle}{\left[1 + \sum_k \frac{|V_k|^2}{(E_j - \omega_k)^2}\right]^{1/2}}, \tag{22}$$

then the residue can be easily interpreted as the amplitude of the bound state in the initial state $|d\rangle$, times the evolution operator of the bound state times the amplitude of the state $|d\rangle$ in the bound state

$$R_j = \langle d\,|E_j\rangle \langle E_j\,|d\rangle e^{-iE_j t}. \tag{23}$$

If the locator has one real pole at E_1, from Eq. (19) we see that the survival probability $p(t) \to |R_1|^2$ when $t \to \infty$. If there are several poles, this equation gives Rabi oscillations.

Notice that Eq. (19) is just the well known result [5]

$$g(t) = \int_{-\infty}^{\infty} A(\omega) e^{-i\omega t} d\omega, \tag{24}$$

where

$$A(\omega) = -\frac{1}{\pi} \mathrm{Im}\left[g(E + is)\right] \tag{25}$$

is the spectral density function. The first term in Eq. (19) is the contribution from the continuous spectrum, and the second term is the contribution from the discrete states.

Before proceeding further, consider two simple models. First model is a site coupled to a semi-infinite lattice. The system is described by the tight-banding Hamiltonian

$$\begin{aligned} H = &-\frac{1}{2}\sum_{n=1}^{\infty}\big(|n\rangle\langle n+1| + |n+1\rangle\langle n|\big) \\ &+\epsilon\,|d\rangle\langle d| - V\big(|d\rangle\langle 1| + |1\rangle\langle d|\big), \end{aligned} \tag{26}$$

where $|n\rangle$ is the state localized at the n-th site of the lattice. The band (lattice) states are described by the Hamiltonian

$$H_0 = -\sum_k \cos k\, |k\rangle\langle k|, \tag{27}$$

where $|k\rangle = \sqrt{2}\sum_n \sin(kn)\ |n\rangle$. Hence we regain Hamiltonian (1) with $V_k = -\sqrt{2}V\sin k$; also

$$\begin{aligned} \Sigma'(E) &= \begin{cases} \Delta_0(E - \mathrm{sign}(E)\sqrt{E^2-1}), & |E| > 1 \\ \Delta_0 E, & |E| < 1 \end{cases} \\ \pi\Delta(E) &= \begin{cases} 0, & |E| > 1 \\ \Delta_0\sqrt{1-E^2}, & |E| < 1 \end{cases}, \end{aligned} \tag{28}$$

where $\Delta_0 = 2V^2$. If we consider the case $\epsilon = 0$ and $V^2/2 < 1$ the locator does not have real poles, so Eq. (12) after substitution of the results of Eq. (28) gives the amplitude of the non-decay amplitude [6]:

$$g(t) = \frac{1}{2\pi}\int_{-\pi}^{\pi} dQ \exp(it\cos Q)\frac{1 - \exp(-2iQ)}{1 + \alpha^2\exp(-2iQ)}, \tag{29}$$

where $\alpha^2 = 1 - \Delta_0$.

For numerical calculations we consider the second model:

$$\Delta(E) = \Delta_0 = \text{const.} \tag{30}$$

The units and zero of energy we'll chose such that $E_b = -1, E_t = 1$; thus we get

$$\Sigma'(E) = \Delta_0 \ln\left|\frac{E+1}{E-1}\right|. \tag{31}$$

There are two real poles of the locator, given by the Equation

$$E - \epsilon - \Delta_0 \ln\left|\frac{E+1}{E-1}\right| = 0. \tag{32}$$

The time we'll measure in units of the FGR time τ

$$1/\tau = 2\pi\Delta_0. \tag{33}$$

For the sake of definiteness we'll chose $\epsilon = -.4$. For $\Delta_0 = .02$ (see Fig. 2) we observe the FGR regime, say, up to $t = 9$. For $\Delta = .1$ (see Fig. 3) the FGR regime

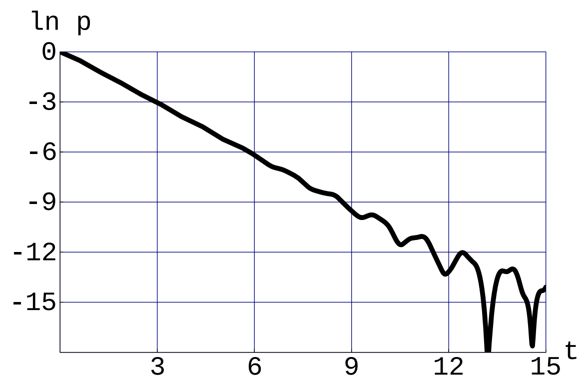


FIG. 2: Survival probability as a function of time for $\Delta_0 = .02$.

is seen up to $t = 3$. For $\Delta_0 = .2$ (see Fig. 4) the FGR

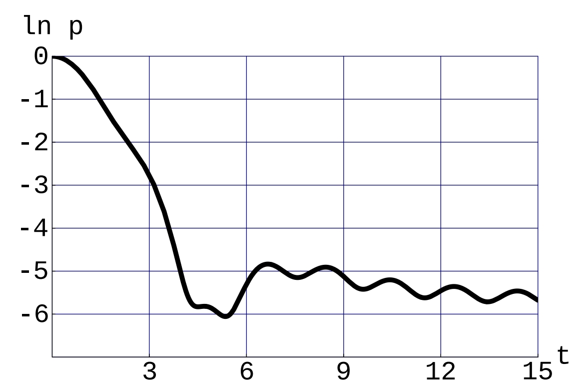


FIG. 3: Survival probability as a function of time for $\Delta_0 = .1$.

regime is absent. The Rabi oscillations we see already at Fig.3 and still more vividly at Fig.4. The FGR is not valid for small t either. (From Eq. (3) it is obvious that the expansion of $g(t)$ is $g(t) = 1 + kt^2 + \ldots$, which gives quadratic decrease of the non-decay probability at small t.) The region of small t, shown at Fig. 5, clearly demonstrates quadratic decrease of p with time.

Let us continue the discussion of what seems to be the (almost) trivial result: FGR at perturbative regime. In fact, in this regime Eq. (16) we could obtain directly

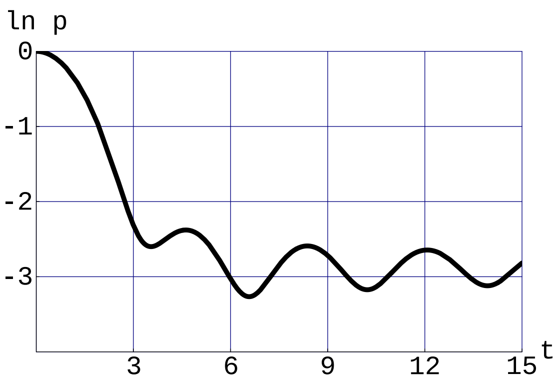


FIG. 4: Survival probability as a function of time for $\Delta_0 = .2$.

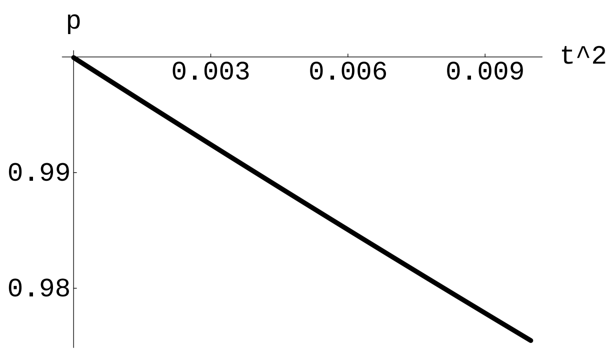


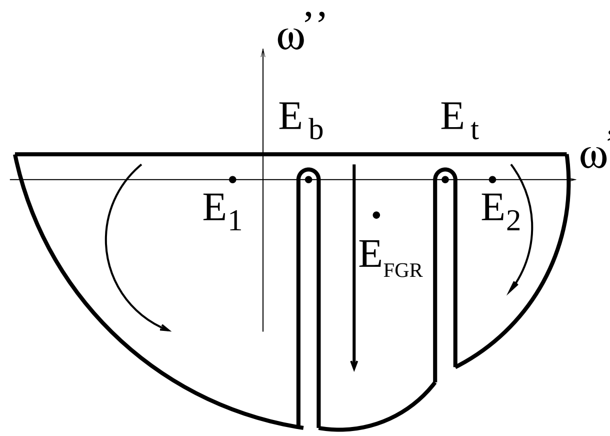
FIG. 5: Survival probability for $\Delta_0 = .02$ (beginning of the process of tunneling).

from Eq. (6), changing exact Green function (7) to an approximate one, which may be called the FGR locator

$$g_{FGR}(\omega) = \frac{1}{\omega - \epsilon - \Sigma'(\epsilon) + i\pi\Delta(\epsilon)}. \tag{34}$$

(Notice, that whichever approximation we use for $\Sigma(\omega)$, the property $a(t=0) = 1$ is protected, provided Σ does not have singularities in the upper half-plane.) Thus approximated, locator has a simple pole $\omega = \epsilon + \Sigma(\epsilon)$, and the residue gives Eq. (16). However, the locator which is used to obtain Eq. (25) and the FGR locator have totally different singularities. So the fact that the locators give the same survival probability (even in finite time interval) demands explanation.

Let us return to the issue of the analytical continuation of the propagator. The examples we considered show that E_b and E_t are the $\Sigma(\omega)$ branch points. Hence propagator is a multi-valued function and it's value in the lower half-plane depends upon the curve along which we continue the function from the upper half-plane [7]. The analytic continuation we used previously, corresponded to continuing $\Sigma(\omega)$ along the curves which circumvent the right branch point clockwise and the and the left branch point anti-clockwise. On the other hand, we could use a different continuation, making the cuts from the branch points to infinity and continuing the function between the cuts along the curves passing through the part of real axis between E_b and E_t, and outside as we did it previously. This way to make analytic continuation, and hence to calculate the integral (6) is presented on Fig. 6. (Of course, the value of the integral does not depend upon the analytic continuation we use.) (The treatment of



[here]

FIG. 6: Alternative way to analytically continue the propagator into the lower half-plane. The arrows show the curves of analytical continuation in between the cuts and outside. Radius of the big arc and length of the cuts go to infinity.

tunneling from the discrete level into a semi-bound continuum presented in the paper by Onley and Kumar [8], corresponds, in fact, to an analytic continuation similar in spirit, to that presented on Fig. 6.) Notice, that because of the exponential decrease as a function of t of the integrand in the cut integrals appearing in this analytic continuation, in contrast to oscillatory behavior of the real axis cut integral, such analytic continuation is more convenient for the numerical calculations of the large t behavior of the non-decay amplitude.

For example, for the model with constant $\Delta(E)$, thus continued self energy is

$$\Sigma(\omega) = \Delta_0 \log\left(\frac{\omega+1}{\omega-1}\right), \tag{35}$$

where log is defined as having the cuts $[-1, -1-i\infty)$ and $[1, 1-i\infty)$, and the phase $-\pi$ at the real axis between -1 and 1. For the model of the semi-infinite chain the relevant self energy sheet is

$$\Sigma(\omega) = \Delta_0\left(\omega - \sqrt{\omega^2 - 1}\right), \tag{36}$$

where the square root is defined as having the phase $\pi/2$ at the real axis between -1 and 1. In both cases the result for $g(t)$ would include the integrals along the cuts presented at Fig. 6.

We can easily understand why the complex pole is present on the sheet of the propagator presented on Fig.

6, but not on that presented on Fig. 1. Consider for simplicity the perturbative regime. In the lower half-plane in the vicinity of $\omega=\epsilon$ the standard propagator is

$$g(\omega)=\frac{1}{\omega-\epsilon-\Sigma'(\epsilon)-i\pi\Delta(\epsilon)}, \tag{37}$$

and the propagator continued according to Fig. 6 is

$$g(\omega)=\frac{1}{\omega-\epsilon-\Sigma'(\epsilon)+i\pi\Delta(\epsilon)}. \tag{38}$$

Thus only the second propagator has (in a perturbative regime) a FGR pole.

CONCLUSIONS

In this paper we solve the problem of tunneling from a discrete level into continuum. We show, how the basic notion of the GF formalism, like frequency dependent discrete level propagator, self energy and spectral density, appear within the basic quantum mechanics. We concentrate on the calculation of the time dependent non-decay amplitude, the stage which is typically not given proper attention to within the GF formalism [5]. We show that the exponential time dependence of the non-decay probability given by the FGR is an approximation valid in perturbative regime and only for intermediate times. The large time dependence of the non-decay probability depends crucially upon the details of the band structure and hybridization interaction. We also look closely at those analytic properties of the propagator in the complex ω plane, which often pass unnoticed.

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APPENDIX

To generalize Eq. (19) to the case of non-interacting Fermi gas at finite temperatures, let us present the Hamiltonian (1) using second quantization

$$H=\sum_k \omega_k c_k^\dagger c_k+\epsilon d^\dagger d+\sum_k\left(V_k c_k^\dagger d+h.c.\right), \tag{39}$$

where $c_k^\dagger(c_k)$ and $d^\dagger(d)$ are creation (annihilation) operators of band states and discrete state respectively. The tunneling of either the electron or the hole from the discrete level into continuum is described by Green's functions $G^>$ and $G^<$ respectively [5]

$$\begin{aligned} G^>(t) &= \left\langle d(t)d^\dagger(0)\right\rangle \\ G^<(t) &= \left\langle d^\dagger(t)d(0)\right\rangle . \end{aligned} \tag{40}$$

where the averaging is with respect to the grand canonical ensemble, and $d(t)$ or $d^\dagger(t)$ is the annihilation or the creation operator in Heisenberg representation. Both Green's functions are simply connected with the spectral density function [5]

$$\begin{aligned} G^>(\omega) &= [1-n_F(\omega)]A(\omega) \\ G^< &= n_F(\omega)A(\omega), \end{aligned} \tag{41}$$

where $n_F(\omega)=\left(e^{\beta(\omega-\mu)}+1\right)^{-1}$ is the Fermi distribution function (μ is the chemical potential and β is the inverse temperature). Thus we obtain

$$\begin{aligned} G^>(t) &= \int_{E_b}^{E_t}\frac{\Delta(E)[1-n_F(E)]e^{-iEt}dE}{[E-\epsilon-\Sigma'(E)]^2+\pi^2\Delta^2(E)} \\ &+ \sum_j[1-n_F(E_j)]R_j \\ G^<(t) &= \int_{E_b}^{E_t}\frac{\Delta(E)n_F(E)e^{-iEt}dE}{[E-\epsilon-\Sigma'(E)]^2+\pi^2\Delta^2(E)} \\ &+ \sum_j n_F(E_j)R_j . \end{aligned} \tag{42}$$

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